JOURNAL OF MOLECULAR STRUCTURE, VOLUME 177 (1988)

AUTHOR INDEX

Ade, 367

Badilescu, S. 69
Balevičius, V. 421
Barnes, A.J. 209
Bogunović, Lj.J. 379
Borgholte, H. 523
Broda, M.A. 351

Chisler, E.V. 231, 531
Chranina, O.V. 309
Colomban, Ph. 277
Czarnik-Matusewicz, B. 359
Czerniakowski, F.P. 309

Davydov, V.Yu. 231
Dega-Szafran, Z. 317
Denisov, G.S. 309
Doucet, J.-P. 407
Dragojević, M.D. 379
Dulewicz, E. 317

Epstein, L.M. 327

Finney, J.L. 23

Gauthier, M. 429
Goethals, G. 407
Goncharuk, I.N. 531
Grech, E. 339

Habermehl, T. 523
Hadjoudis, E. 191
Hadži, D. 1
Hawranek, J.P. 351, 359
Hermann, A. 367
Hoffmann, V. 367

Ichikawa, M. 441
Iskanderov, T.A. 221
Ito, M. 173
Itoh, R. 449

Khan, A. 543
Kimel'fel'd, Ya.M. 221
Kimtys, L. 421
Kleeberg, H. 157
Kravtsov, D.N. 327
Kreuer, K.-D. 265
Kristiansson, O. 537
Kroon, J. 467

Le-Thanh, H. 69
Limbach, H.-H. 143
Lindgren, J. 537
Luck, W.A.P. 523

Malarski, Z. 339
Maršalka, A. 421
Meschede, L. 143
Milia, F. 191
Mioč, U.B. 379
Mordziński, A. 385
Moreau Descoings, M.-C. 407
Nagy, O.B. 393
Novak, A. 277

Parbhoo, B. 393
Pawlak, Z. 401
Pruzan, Ph. 429

Ratajczak, H. 487
Ribnikar, S.V. 379
Rumpel, H. 143

Saitoh, T. 449
Sandorfy, C. 69
Savage, H.F.J. 23
Saval'ev, V.A. 93
Scheiner, S. 79
Scherer, G. 143
Schlabach, M. 143
Schmidt, V.H. 257
Scott, R.M. 513, 543
Seguin, J.-P. 407
Seliger, J. 191
Shubina, E.S. 327
Slanina, Z. 459
Smirnova, E.M. 221
Sobczyk, L. 111, 339
Sokolov, N.D. 93
Stouten, P.F.W. 467
Szafran, M. 317

Tarakanova, E.G. 495
Thomas, R. 513
Tomoda, S. 199

Urbańczyk, G. 401

Vener, M.V. 93
Videnova-Adrabińska, V. 477
Vocelle, D. 69

Walker, G. 513
Waluk, J. 415
Wehrle, B. 143
Weiss, J. 367
White, D. 513
Wierzejewska Hnat, M. 487

Yazdani, S. 513
Ye, Z. 513
Yukhnevich, G.V. 495

Zeegers-Huyskens, T. 126
Zundel, G. 43

JOURNAL OF MOLECULAR STRUCTURE, VOLUME 177(1988)

SUBJECT INDEX

Acetonitrile,
formation of $(NHN_1)^+$ hydrogen bonded cations in acetonitrile 401
Acidity,
cooperative effects in H-bond formation: influence on the acidity of proton donors 157
Acid tetrahedron groups H_nAsO_4 (n=1-3),
H-bond length dependence of the distortion in acid tetrahedron groups H_nAsO_4 (n=1-3) 441
Alcohols,
IR bandshapes of weakly H-bonded complexes of tertiary alcohols with oxygen bases 359
Amines,
short range solvation effects with primary and secondary amines 513
2-Aminopyridine dimers,
luminescence of hydrogen-bonded 2-aminopyridine dimers 415
Ammonia,
internal Raman spectrum of ammonia up to 75 GPa suggesting the loss of the molecular character above about 60 Gpa 429
Angular characteristics,
relationship between the angular characteristics of a hydrogen bond and the energetics of proton transfer occurring within 79
Anilines,
hydrogen bonded solvation structures in the reaction of carboxylic acides and anilines in cyclohexane acetic acid solutions 543

Benzoxazoles,
proton transfer reaction in the electronically excited H-bonded benzoxazoles 385
Biological mechanisms,
proton transfers in biological mechanisms 1
Biological systems,
proton transfer in and proton polarizability of hydrogen bonds: IR and theoretical studies regarding mechanisms in biological systems 43
Biomolecule crystal hydrates,
impenetrability revisited: new light on hydrogen bonding from neutron studies on biomolecule crystal hydrates 23

Carboxylic acids,
hydrogen bonded solvation structures in the reaction of carboxylic acids and anilines in cyclohexane acetic acid solutions 543
Charge distribution,
charge distribution and proton transfer in hydrogen bonded complexes 111
Chloroacetic acid,
interaction of 2,6-dimethylpyridine with chloroacetic acid in some aprotic solvents: problem of stoichiometry 317
Cooperative effects,
cooperative effects in H-bond formation: influence on the acidity of proton donors 157
Cyclohexane acetic acid solutions,
hydrogen bonded solvation structures in the reaction of carboxylic acids and anilines in cyclohexane acetic acid solutions 543

2,6-Dichloro-4-nitrophenol,
vibrational dephasing of ν_s (OH) in 2,6-dichloro-4-nitrophenol 351
2,6-Dimethylpyridine,
interaction of 2,6-dimethylpyridine with chloroacetic acid in some aprotic solvents: problem of stoichiometry 317

Energetics of proton transfer,
relationship between the angular characteristics of a hydrogen bond and the energetics of proton transfer occurring within 79
Exponential expression,
importance of the proton affinities in hydrogen bond studies. A new exponential expression 125

F^- anion,
on the hydration of the F^- anion in aqueous solution 537

Fast proton transport,
fast proton transport in solids 265
Ferroelectric KD_2PO_4,
Raman study of the low frequency deuteronic vibrations in ferroelectric KD_2PO_4 531
Ferroelectrics,
spectroscopic manifestation of the short hydrogen bonds in KH_2PO_4 type ferroelectrics 231

Hydrogen dichloride ion, $(ClHCl)^-$,
ab inito SCF-SDCI prediction of type II spectra and geometry of hydrogen dichloride ion, $(ClHCl)^-$ 449
Hydrogen fluoride dimer,
ionic state of the hydrogen fluoride dimer: equilibrium structure $HFH^+\cdots F$ and its dissociation energies for the protonation and non-protonation channels 199
Hydrophilic-hydrophobic interactions,
molecular dynamics in hydrogen bond forming environments. The role of hydrophilic-hydrophobic interactions in pyridine-water mixtures 393
Hydroxylic compounds,
^{13}C NMR measurement of hydrogen bonding effects for hydroxylic compounds: relationships between the OH stretching frequencies, the chemical shifts of proton donor group and electron reorganization 407

In concreto and in computro,
hydrogen bonds in concreto and in computro 467
Isostructural systems,
hydrogen and coordination bonds in isostructural systems. Are hydrogen bonds unique? 327
Isotope effects,
tentative study of the strong hydrogen bond dynamics. Part I. Geometric isotope effects 93

Ketonic solvents,
investigation of the hydrogen bonding of triphenylcarbinol and triphenylsilanol in ketonic solvents by means of infrared spectroscopy 379
KH_2PO_4,
spectroscopic manifestation of the short hydrogen bonds in KH_2PO_4 type ferroelectrics 231

Liquid crystals,
high resolution ^1H NMR studies of hydrogen bonding in liquid crystals 421
Low-temperature matrices,
infrared photochemistry of hydrogen-bonded complexes trapped in low-temperature matrices 209

Methanol-water mixtures
H-bonds in methanol-water mixtures: indications of non-H-bonded OH in liquid water 523
Multiple proton transfers,
NMR and IR studies of novel multiple proton transfers in liquids, crystals, and organic glasses 143

Neutron studies,
impenetrability revisited: new light on hydrogen bonding from neutron studies on biomolecule crystal hydrates 23
$(NH_4)_2HPO_4$ single crystal,
the hydrogen bond in the monoclinic $(NH_4)_2HPO_4$ single crystal 477
NHN hydrogen bonds,
structure and IR spectroscopic behaviour of NHN hydrogen bonds 339
Noble gases,
infrared spectra of hydrogen bonded complexes in solutions of noble gases 221

Potential energy surface,
some properties of the potential energy surface and vibrational spectrum of a strong hydrogen bond complex 495
Proton glasses,
proton transfer in proton glasses 257
Pyridine-water mixtures,
molecular dynamics in hydrogen bond forming environments. The role of hydrophilic-hydrophobic interactions in pyridine-water mixtures 393
Pyrrole-pyridine complexes,
nuclear magnetic relaxation and rotational diffusion of pyrrole-pyridine complexes 367

Retinal Schiff base,
attenuated total reflection FTIR study of the protonation of a retinal Schiff base 69

N-Salicylidene anilines,
hydrogen bond studies in thermochromic and photochromic *N*-salicylidene anilines 191
Strong hydrogen bond complex,
some properties of the potential energy surface and vibrational spectrum of a strong bond complex 495
Strong hydrogen bond dynamics,
tentative study of the strong hydrogen bond dynamics. Part I. Geometric isotope effects 93
Superionic conductivity,
proton transfer and superionic conductivity in solids and gels 277
Supersonic jet spectroscopy,
supersonic jet spectroscopy for the study of hydrogen bonding 173
Trichloromethane–base,
matrix isolation infrared studies of trichloromethane–base complexes 487
Triphenylcarbinol and triphenylsilanol, investigation of the hydrogen bonding of triphenylcarbinol and triphenylsilanol in ketonic solvents by means of infrared spectroscopy 379

UV-vis electrochromism,
UV-vis electrochromism due to proton transfer 309

Water clusters,
theoretical studies of water clusters and consequences for gas-phase and liquid water 459
Water,
H-bonds in methanol–water mixtures: indications on non-H-bonded OH in liquid water 523

CONTENTS

Preface ..... *xi*

Proton transfers in biological mechanisms
D. Hadži (Ljubljana, Yugoslavia) 1
Impenetrability revisited: new light on hydrogen bonding from neutron studies on biomolecule crystal hydrates
J.L. Finney (London, Gt. Britain and H.F.J. Savage (New York, NY, U.S.A.) 23
Proton transfer in and proton polarizability of hydrogen bonds: IR and theoretical studies regarding mechanisms in biological systems
G. Zundel (München, F.R.G.) 43
Attenuated total reflection FTIR study of the protonation of a retinal Schiff base
S. Badilescu, C. Sandorfy, H. Le-Thanh and D. Vocelle (Montréal, Qué., Canada) 69
Relationship between the angular characteristics of a hydrogen bond and the energetics of proton transfer occurring within
S. Scheiner (Carbondale, IL, U.S.A.) 79
Tentative study of the strong hydrogen bond dynamics. Part I. Geometric isotope effects
N.D. Sokolov, M.V. Vener and V.A. Saval'ev (Moscow, U.S.S.R.) 93
Charge distribution and proton transfer in hydrogen bonded complexes
L. Sobczyk (Wrocław, Poland) 111
Importance of the proton affinities in hydrogen bond studies. A new exponential expression
Th. Zeegers-Huyskens (Heverlee, Belgium) 125
NMR and IR studies of novel multiple proton transfers in liquids, crystals, and organic glasses
H.-H. Limbach, H. Rumpel, L. Meschede, B. Wehrle, M. Schlabach and G. Scherer (Freiburg, F.R.G.) 143
Cooperative effects in H-bond formation: influence on the acidity of proton donors
H. Kleeberg (Marburg, F.R.G.) 157
Supersonic jet spectroscopy for the study of hydrogen bonding
M. Ito (Sendai, Japan) 173
Hydrogen bond studies in thermochromic and photochromic *N*-salicylidene anilines
F. Milia, E. Hadjoudis (Athens, Greece) and J. Seliger (Ljubljana, Yugoslavia) 191
Ionic state of the hydrogen fluroide dimer: equilibrium structure $HFH^+ \cdots F$ and its dissociation energies for the protonation and non-protonation channels
S. Tomoda (Osaka, Japan) 199
Infrared photochemistry of hydrogen-bonded complexes trapped in low-temperature matrices
A.J. Barnes (Salford, Gt. Britain) 209
Infrared spectra of hydrogen bonded complexes in solutions of noble gases
T.A. Iskanderov, Ya.M. Kimel'fel'd and E.M. Smirnova (Moscow, U.S.S.R.) 221
Spectroscopic manifestation of the short hydrogen bonds in KH_2PO_4 type ferroelectrics
E.V. Chisler and V. Yu, Davydov (Leningrad, U.S.S.R.) 231
Proton transfer in proton glasses
V.H. Schmidt (Bozeman, MT, U.S.A.) 257
Fast proton transport in solids
K.-D. Kreuer (Stuttgart, F.R.G.) 265
Proton transfer and superionic conductivity in solids and gels
Ph. Colomban (Palaiseau, France) and A. Novak (Thiais, France) 277
UV-Vis electrochromism due to proton transfer
O.V. Chranina, F.P. Czerniakowski and G.S. Denisov (Leningrad, U.S.S.R.) 309
Interaction of 2,6-dimethylpyridine with chloroacetic acid in some aprotic solvents: problem of stoichiometry

Z. Dega-Szafran, E. Dulewicz and M. Szafran (Poznan, Poland) 317
Hydrogen and coordination bonds in isostructural systems. Are hydrogen bonds unique?
L.M. Epstein, E.S. Shubina and D.N. Kravtsov (Moscow, U.S.S.R.) 327
Structure and IR spectroscopic behaviour of NHN hydrogen bonds
Z. Malarski, L. Sobczyk (Wroclaw, Poland) and E. Grech ((Szczecin, Poland) 339
Vibrational dephasing of ν_s (OH) in 2,6-dichloro-4-nitrophenol
M.A. Broda and J.P. Hawranek (Wroclaw, Poland) 351
IR bandshapes of weakly H-bonded complexes of tertiary alcohols with oxygen bases
B. Czarnik-Matusewicz and J.P. Hawranek (Wroclaw, Poland) 359
Nuclear magnetic relaxation and rotational diffusion of pyrrole–pyridine complexes
T. Ade, A. Hermann, V. Hoffmann and J. Weiss (Tübingen, F.R.G.) 367
Investigation of the hydrogen bonding of triphenylcarbinol and triphenylsilanol in ketonic solvents by means of infrared spectroscopy
U.B. Mioč, Lj.J. Bogunović, S.V. Ribnikar and M.D. Dragojević (Belgrade, Yugoslavia) 379
Proton transfer reaction in the electronically excited H-bonded benzoxazoles
A. Mordziński (Kasprzaka, Poland) 385
Molecular dynamics in hydrogen bond forming environments. The role of hydrophilic–hydrophobic interactions in pyridine–water mixtures
B. Parbhoo and O.B. Nagy (Louvain-la-Neuve, Belgium) 393
Formation of $(NHN_1)^+$ hydrogen bonded cations in acetonitrile
Z. Pawlak and G. Urbańczyk (Sopot, Poland) 401
^{13}C NMR measurement of hydrogen bonding effects for hydroxylic compounds: relationships between the OH stretching frequencies, the chemical shifts of proton donor group and electron reorganization
M.-C., Moreau Descoings, G. Goethals, J.-P. Seguin (Amiens, France) and J.-P. Doucet (Paris, France) 407
Luminescence of hydrogen-bonded 2-aminopyridine dimers
J. Waluk (Kasprzaka, Poland) 415
High resolution ^1H NMR studies of hydrogen bonding in liquid crystals
V. Balevičius, A. Maršalka and L. Kimtys (Vilnius, U.S.S.R.) 421
Internal Raman spectrum of ammonia up to 75 GPa suggesting the loss of the molecular character above about 60 GPa
Ph. Pruzan and M. Gauthier (Paris, France) 429
H-bond length dependence of the distortion in acid tetrahedron groups H_nAsO_4 (n= 1–3)
M. Ichikawa (Sapporo, Japan) 441
Ab initio 3CF-SDCI prediction of type II spectra and geometry of hydrogen dichloride ion, $(ClHCl)^-$
T. Saitoh and R. Itoh (Tokyo, Japan) 449
Theoretical studies of water clusters and consequences for gas-phase and liquid water
Z. Slanina (Prague, Czechoslovakia) 459
Hydrogen bonds in concreto and in computro
P.F.W. Stouten and J. Kroon (Utrecht, The Netherlands) 467
The hydrogen bond in the monoclinic $(NH_4)_2HPO_4$ single crystal
V. Videnova-Adrabińska (Wroclaw, Poland) 477
Matrix isolation infrared studies of trichloromethane–base complexes
M. Wierzejewska Hnat and H. Ratajczak (Wroclaw, Poland) 487
Some properties of the potential energy surface and vibrational spectrum of a strong hydrogen bond complex
G.V. Yukhnevich and E.G. Tarakanova (Moscow, U.S.S.R.) 495
Short range solvation effects with primary and secondary amines
Z. Ye, S. Yazdani, R. Thomas, G. Walker, D. White and R.M. Scott (Ypsilanti, MI, U.S.A.) 513
H-bonds in methanol–water mixtures: indications of non-H-bonded OH in liquid water
W.A.P. Luck, H. Borgholte and T. Habermehl (Marburg, F.R.G.) 523

Raman study of the low frequency deuteronic vibrations in ferroelectric KD_2PO_4
I.N. Goncharuk and E.V. Chisler (Leningrad, U.S.S.R.) 531
On the hydration of the F^- anion in aqueous solution
O. Kristiansson and J. Lindgren (Uppsala, Sweden) 537
Hydrogen bonded solvation structures in the reaction of carboxylic acids and anilines in cyclohexane acetic acid solutions
A. Khan and R.M. Scott (Ypsilanti, MI, U.S.A.) 543

Author Index 551
Subject Index 553